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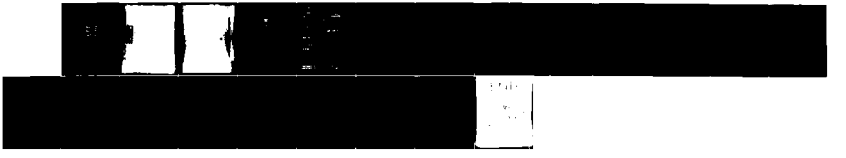

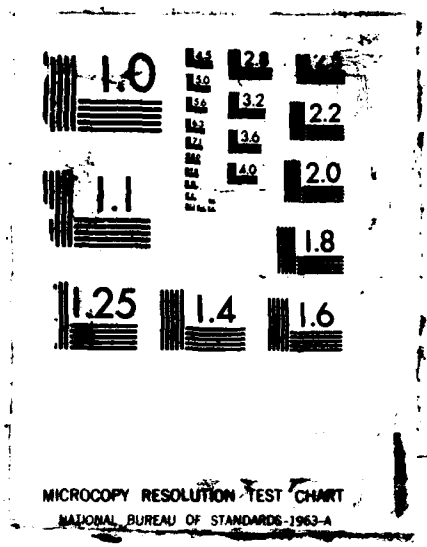
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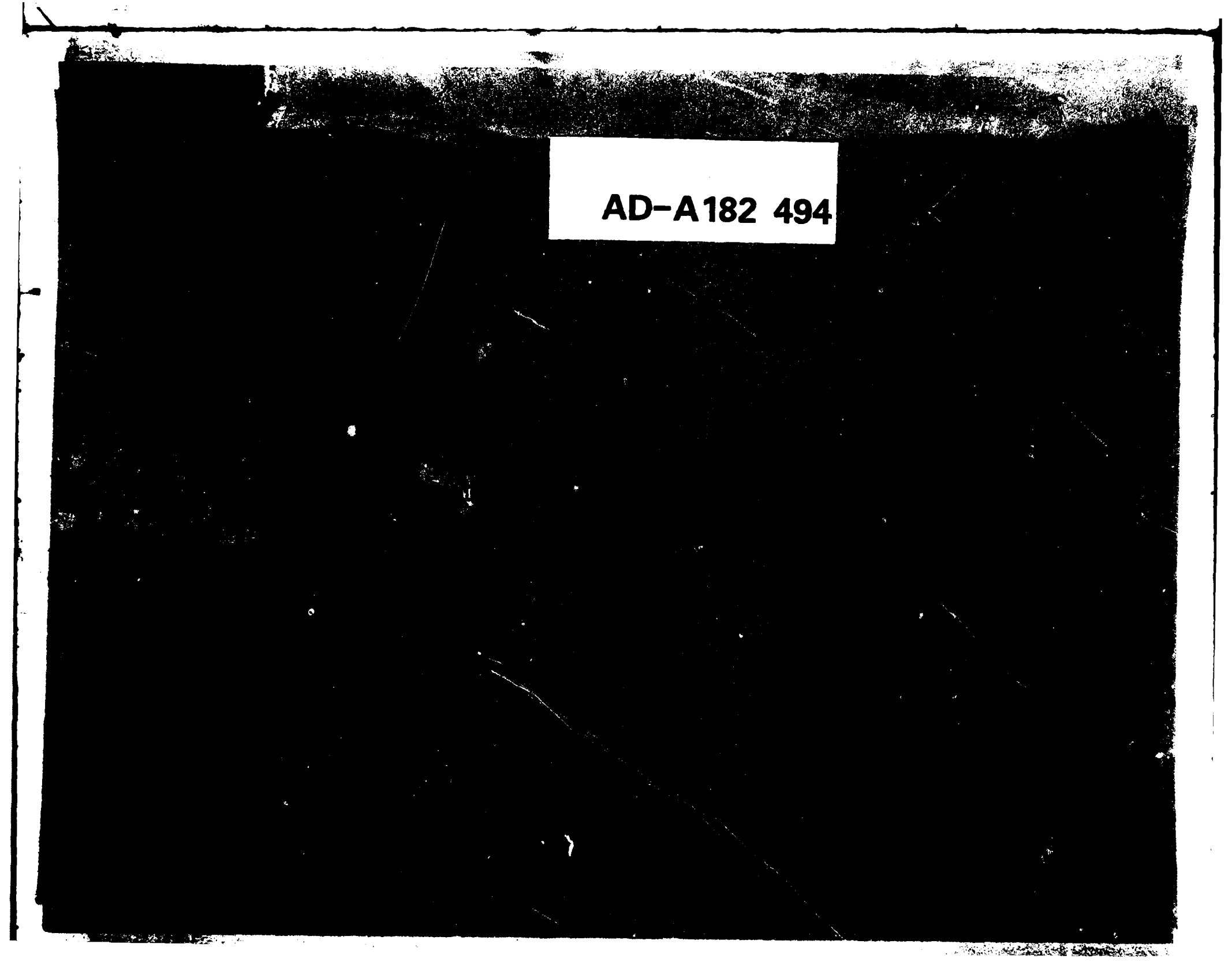

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PREFACE

I prepared this project as an article for publication. I wrote it in the style of the target journal which explains the use of double spacing, the heavy use of passive voice, and the unusual format for the references. Subject to clearance, this manuscript will be submitted to The International Journal for Numerical Methods in Engineering for consideration.

There are parallel methods for solving parabolic differential equations in both finite elements and finite differences. Quite often, the method of choice for treating the temporal domain is the Crank-Nicolson method. A closely related method for finite differences is the Crandall method. Similarities between the matrix equations for the Crank-Nicolson versions of finite differences and finite elements suggested searching for an equivalent for the Crandall method for finite elements. I found such a method to exist, and it is derived herein. I have also provided a theoretical treatment of accuracy and stability along with numerical results for validation.

ABOUT THE AUTHOR

Charles R. Martin was born on 25 September, 1950 in Wiesbaden, Germany, the son of Clyde J. Martin and Lillian R. Martin. Upon completion of high school at Watauga High School, Boone, North Carolina in 1968, he entered North Carolina State University at Raleigh, Raleigh, North Carolina where he was enrolled in a cooperative education program in Nuclear Engineering. His cooperative work was performed with the Nuclear Division of Duke Power Company, Charlotte, North Carolina. In May of 1973, he was graduated with Honors as a Bachelor of Science in Nuclear Engineering. Concurrently, he completed the Reserve Officers Training Corps program as a Distinguished Graduate. In November of 1973, he completed Missile Combat Crew Operational Readiness Training at Vandenburg AFB, California as a Distinguished Graduate of that program. For the next three years, he served as a Deputy Missile Combat Crew Commander and Missile Launch Procedures Instructor at Malmstrom AFB, Montana. In March of 1978, he was graduated with Distinction with a Master of Science in Nuclear Engineering by the Air Force Institute of Technology, Wright-Patterson AFB, Ohio. He then served for two years as an Instructor and Course Director in the Department of Mathematical Sciences at the United States Air Force Academy in Colorado. In June of 1980, he was awarded a fellowship from the Air Force Academy to attend the Air Force Institute of Technology for a Doctor of Philosophy degree in Nuclear Engineering with a minor in Mathematics. Upon graduation, he was sent to the Defense Nuclear Agency as a Technical Director for underground nuclear weapons testing at the Nevada Test Site where he conducted 3 nuclear tests and 13 high explosive tests. He is presently attending the Air Command and Staff College at Maxwell AFB, Alabama.

AN OPTIMUM FORMULATION OF THE FINITE ELEMENT METHOD FOR THE DIFFUSION EQUATION

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SUMMARY

An optimum formulation of the finite element method for the diffusion equation is derived and applied to a problem with Dirichlet and Neumann boundary conditions. The method is the finite element analog of the Crandall method[1] for finite differences.

INTRODUCTION

In an earlier paper, the Crandall (CM) and Crank-Nicolson (CNM) finite difference methods were compared[2] with respect to the solution of the transient heat conduction problem (isomorphic with respect to the diffusion equation).

In this paper, an optimum formulation of the finite element method (FEM) for the diffusion equation is derived. This method is the finite element equivalent of the Crandall method for finite differences. The method is then applied to problems with Neumann and Dirichlet boundary conditions, and the accuracy is compared with the finite element version of the CNM.

DERIVATION OF THE METHOD

The following quadratic functional, given by Myers,[3]

$$I(\phi) = \int_0^1 \left[\left(\frac{\partial \phi}{\partial x}\right)^2 + \frac{\partial}{\partial \theta}\,\phi^2\right] dx \tag{1}$$

is related to the normalized diffusion equation

$$\frac{\partial \phi}{\partial \theta} = \frac{\partial^2 \phi}{\partial x^2}$$

with boundary conditions

$$\phi(0,\ \theta) = 0\ ,\ \theta > \tilde{0} \tag{2}$$

$$\left.\frac{\partial \phi}{\partial x}\right|_{x=1} = 0\ ,\ \theta > 0$$

and initial condition

$$\phi(x,\ 0) = 1$$

where

ϕ is the normalized flux
θ is the normalized time variable
x is the normalized space variable

by the fact that

$$I(\phi) \leq I(\tilde{\phi}) \text{ for all } \tilde{\phi} \text{ in } H_E^1 \tag{3}$$

where ϕ is the solution to equation (2) and where H_E^1, the solution space for equation (2), is a Hilbert space in which the member functions and their first derivatives are square integrable and which satisfy the essential boundary condition of equation (2).

In practice, a solution is sought within a finite dimensional subspace of H_E^1. This solution will be the Ritz

projection of the true solution onto the subspace S^E, where the superscript E indicates the number of elements used in the finite element solution.

The elements of S^E are the trial functions, $\tilde{\phi}^E$. Since they belong to H_E^1, they satisfy

$$\tilde{\phi}^E(0, \theta) = 0 \ , \ \theta > 0 \tag{4}$$

The simplest choice for the functions $\tilde{\phi}^e$ are functions which are linear within each element, continuous at the elemental interfaces, and zero at x = 0. Thus $\tilde{\phi}^E$ is expanded in terms of the familiar tent functions (θ held fixed):

$$\tilde{\phi}^E(x) = \tilde{\phi}_1 + \sum_{e=1}^{E} \tilde{\phi}_e \, T_e^E(x) \tag{5}$$

where $T_e^E(x)$ varies linearly from $(e-1)\,\Delta x$ to $e\Delta x$, is equal to unity at $e\Delta x$, varies linearly from $e\Delta x$ to $(e+1)\Delta x$, and is equal to zero at all other points on the domain including $(e-1)\,\Delta x$ and $(e+1)\Delta x$. The interval spacing is taken to be constant, thus $\Delta x = 1/E$.

The problem, then, is to minimize

$$I(\tilde{\phi}^e) = \int_0^1 \left[\left(\frac{\partial \tilde{\phi}^e}{\partial x} \right)^2 + \frac{\partial}{\partial \theta} (\tilde{\phi}^e)^2 \right] dx \tag{6}$$

over a single element, then

$$\int_{(e-1)\Delta x}^{e\Delta x} \left[\left(\frac{\partial \tilde{\phi}^e}{\partial x} \right)^2 + \frac{\partial}{\partial \theta} (\tilde{\phi}^e)^2 \right] dx$$

$$= \left[\tilde{\phi}_{e-1} \ \tilde{\phi}_e \right] \underline{k} \begin{bmatrix} \tilde{\phi}_{e-1} \\ \tilde{\phi}_e \end{bmatrix} + \frac{\partial}{\partial \theta} \left[\tilde{\phi}_{e-1} \ \tilde{\phi}_e \right] \underline{m} \begin{bmatrix} \tilde{\phi}_{e-1} \\ \tilde{\phi}_e \end{bmatrix} \tag{7}$$

where $\underline{k}^e = \frac{1}{\Delta x} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$ is the element stiffness matrix, and

$\underline{m}^e = \frac{\Delta x}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$ is the element mass matrix. For the whole interval then

$$\int_0^1 \left[\left(\frac{\partial \tilde{\phi}^e}{\partial x}\right)^2 + \frac{\partial}{\partial \theta}\left(\tilde{\phi}^e\right)^2\right] dx$$

$$= \sum_{e=1}^{E} \left[\begin{bmatrix} \tilde{\phi}_{e-1} & \tilde{\phi}_e \end{bmatrix} \underline{K}^e \begin{bmatrix} \tilde{\phi}_{e-1} \\ \tilde{\phi}_e \end{bmatrix} + \frac{\partial}{\partial \theta} \begin{bmatrix} \tilde{\phi}_{e-1} & \tilde{\phi}_e \end{bmatrix} \underline{M}^e \begin{bmatrix} \tilde{\phi}_{e-1} \\ \tilde{\phi}_e \end{bmatrix} \right]$$

$$= \underline{\tilde{\phi}}^T \underline{K}\, \underline{\tilde{\phi}} + \frac{\partial}{\partial \theta}\, \underline{\tilde{\phi}}^T \underline{M}\, \underline{\tilde{\phi}} \qquad (8)$$

where $\underline{\tilde{\phi}}^T = [\tilde{\phi}_1\ \tilde{\phi}_2\ \cdots\ \tilde{\phi}_E]$, $\underline{K}$ is the global stiffness matrix, and $\underline{M}$ is the global mass matrix. The minimum occurs at the point $\partial I/\partial \tilde{\phi}_j = 0$ for the vector $\underline{\phi}^T = [\phi_1\ \phi_2\ \cdots\ \phi_E]$ determined by

$$\underline{M}\, \frac{\partial}{\partial \theta}\, \underline{\phi} + \underline{K}\ \underline{\phi} = 0 \qquad (9)$$

If equation (9) is approximated by the Crank-Nicolson scheme,[4] the result is

$$\underline{M}\left(\frac{\underline{\phi}^{k+1} - \underline{\phi}^k}{\Delta t}\right) + \underline{K}\ \left(\frac{\underline{\phi}^{k+1} + \underline{\phi}^k}{2}\right) = 0 \qquad (10)$$

An optimum formulation can be derived if a more general form of equation (10) is assumed

$$(\underline{M} + \underline{K}\,\alpha\Delta t)\ \underline{\phi}^{k+1} = (\underline{M} - \underline{K}(1-\alpha)\,\Delta t)\ \underline{\phi}^k \qquad (11)$$

where the parameter α represents the weight placed on the next time level, k+1. While the L_∞ norm is not a natural one for the finite element method, it is of interest to investigate the error with respect to that norm. If the set of equations represented

by equation (11) are treated as difference equations, then the inherent truncation error can be investigated by representing the exact solution to $\phi_{xx} = \phi_{\theta}$ at adjacent points in the space time network by means of Taylor's series centered at $(i\Delta x, k\Delta\theta)$. When these are substituted into the general expression

$$A_1 \phi_{i-1,k+1} + A_2 \phi_{i,k+1} + A_1 \phi_{i+1,k+1} = B_1 \phi_{i-1,k} + B_2 \phi_{i,k} + B_1 \phi_{i+1,k} \tag{12}$$

where

$$A_1 = 1-6\alpha p$$
$$A_2 = 4+12\alpha p$$
$$B_1 = 1+6(1-\alpha)p$$
$$B_2 = 4-12(1-\alpha)p$$
$$p = \Delta\theta/(\Delta x)^2$$

(p is known within the literature as the Fourier modulus) then the remainder terms of the Taylor's series are

$$\Delta x^2\left(\frac{p}{2} - \alpha p + \frac{1}{12}\right)\phi_{\theta\theta} + \Delta x^4 \left[p^2(1-3\alpha) + \left(p\left(\frac{1}{2} - \frac{\alpha}{2}\right) + \frac{1}{15}\right)\phi_{\theta\theta\theta}\right] + 0(\Delta x^6) + \cdots \tag{13}$$

where the identities

$$\phi_{\theta\theta} = \phi_{\theta xx} = \phi_{xxxx} \tag{14}$$
$$\phi_{\theta\theta\theta} = \phi_{\theta\theta xx} = \phi_{\theta xxxx} = \phi_{xxxxxx}$$

have been used. It is obvious that the expression (11) is $0(\Delta x^2)$ accurate at the nodes. An $0(\Delta x^4)$ scheme can be derived by setting the coefficient of the $0(\Delta x^2)$ term to zero. Thus when

$$\alpha = \frac{1}{2}\left(1 + \frac{1}{6p}\right) \tag{15}$$

is satisfied, equation (11) is $0(\Delta x^4)$ accurate at the nodes. Furthermore, at the intersection point of the $0(\Delta x^2)$ and $0(\Delta x^4)$ terms, that is at the point

$$\alpha = \frac{\sqrt{5}}{10}$$

$$p = \frac{3 + \sqrt{5}}{6}$$

the truncation error of (13) and therefore of (11) is $0(\Delta x^6)$.

The stability of the method can be easily investigated for a pure Dirichlet problem by noting that equation (11) can be written as

$$\underline{A}\ \underline{\phi}^{k+1} = \underline{B}\ \underline{\phi}^{k} \tag{16}$$

In this formulation, the first and last equations in the system may be dropped, thus eliminating the known boundary values and reducing the number of unknowns by two. These changes will not alter the numerical solution. In the resulting system, $\underline{A}$ and $\underline{B}$ are tridiagonal. Smith[5] gives the eigenvalues for the iteration matrix $\underline{C} = \underline{A}^{-1}\underline{B}$ as

$$(\lambda_C)_n = \frac{(1+2p\alpha) + 2(-p\alpha)\cos\frac{n\pi}{N+1}}{(1+2p(1\alpha)) + 2(p(1-\alpha))\cos\frac{n\pi}{N+1}} \tag{17}$$

where N is the number of equations. The analysis will be done for the limiting case where $N \to \infty$, that is, for a large system of

equations. The eigenvalues for a system of 40 equations are very close to the limiting values. The eigenvalues of such a system are bounded above by one. The minimum eigenvalue then will control the stability of the system and is given when n = N by

$$(\lambda_c)_\infty = \frac{1+12p\alpha}{1-12\ p(1-\alpha)} \tag{13}$$

Since α gives the "degree of implicitness" of equation (11), the entire family of finite element expressions can be investigated. Figure 1 shows graphically the results of the analysis for the pure-implicit, optimum-implicit, Crank-Nicolson, and explicit (Euler) formulations. It is immediately obvious that the optimum-implicit method is more stable than the Crank-Nicolson method. This is not the case with finite differences.

RESULTS

Extensive calculations were made using equations (11) and (15). Due to the discontinuity in the boundary condition at t = 0 and x = 0, problems with respect to convergence of the numerical solution were encountered. This was true also with the Crandall method, however. To eliminate the problems owing to the discontinuity, the exact analytical solution to equation (1) was substituted for the numerical solution at the end of the first time step. The convergence of the numerical solution after a change in the discretization scheme from 10 to 20 elements is shown in Figure 2. The discretization error ratio (DER) is defined as the total error between the exact and numerical

solutions for E elements divided by the error at the same point when E has been doubled. Here the truncation error has been summed over all 9 internal nodes for the 10 element discretization scheme and the corresponding 9 internal nodes for the 20 element scheme and is termed "generalized mean error." In Figure 2, the DER is graphed as a function of time for three values of the parameter α, while in Figure 3, it is graphed as a function of α for three points in time. The elemental truncation error for the Crank-Nicolson method ($\alpha = .5$) and the pure-implicit method ($\alpha = 1.0$) is approximately 1/4 if Δx is halved. For the optimum formulation given here, the elemental truncation error is approximately 1/16 if Δx is halved. It is clear from Figure 2 that all three methods approach their theoretical improvement ratios. It is also interesting to note that the H^0 error norm, defined by

$$||\phi - \phi^E||_0 = \int_0^1 (\phi - \phi^E)^2 \, dx \tag{19}$$

shows a peak structure in Figure 4 similar to that observed for the truncation error shown in Figure 3. This observation leads to speculation that there may be a predictable value of α which optimizes the finite element system (11) with respect to the H^0 error norm.

CONCLUSIONS

1. The optimum method derived here using linear finite elements yields the same system of equations as the Crandall method for

pure finite differences. The finite element solution is continuous, however, rather than discrete.

2. The stability for the optimum-implicit scheme is greater than for the Crank-Nicolson method since the oscillation limits are less restrictive than in the latter method.

3. The theoretical increase in accuracy for the optimum method over the Crank-Nicolson method is clearly verified by the numerical results.

4. The discontinuity in the boundary condition at $t = 0$, $x = 0$ for the Neumann problem causes a loss in the order of convergence which may be recoverable by using a discontinuous elemental trial function at the point of the discontinuity.

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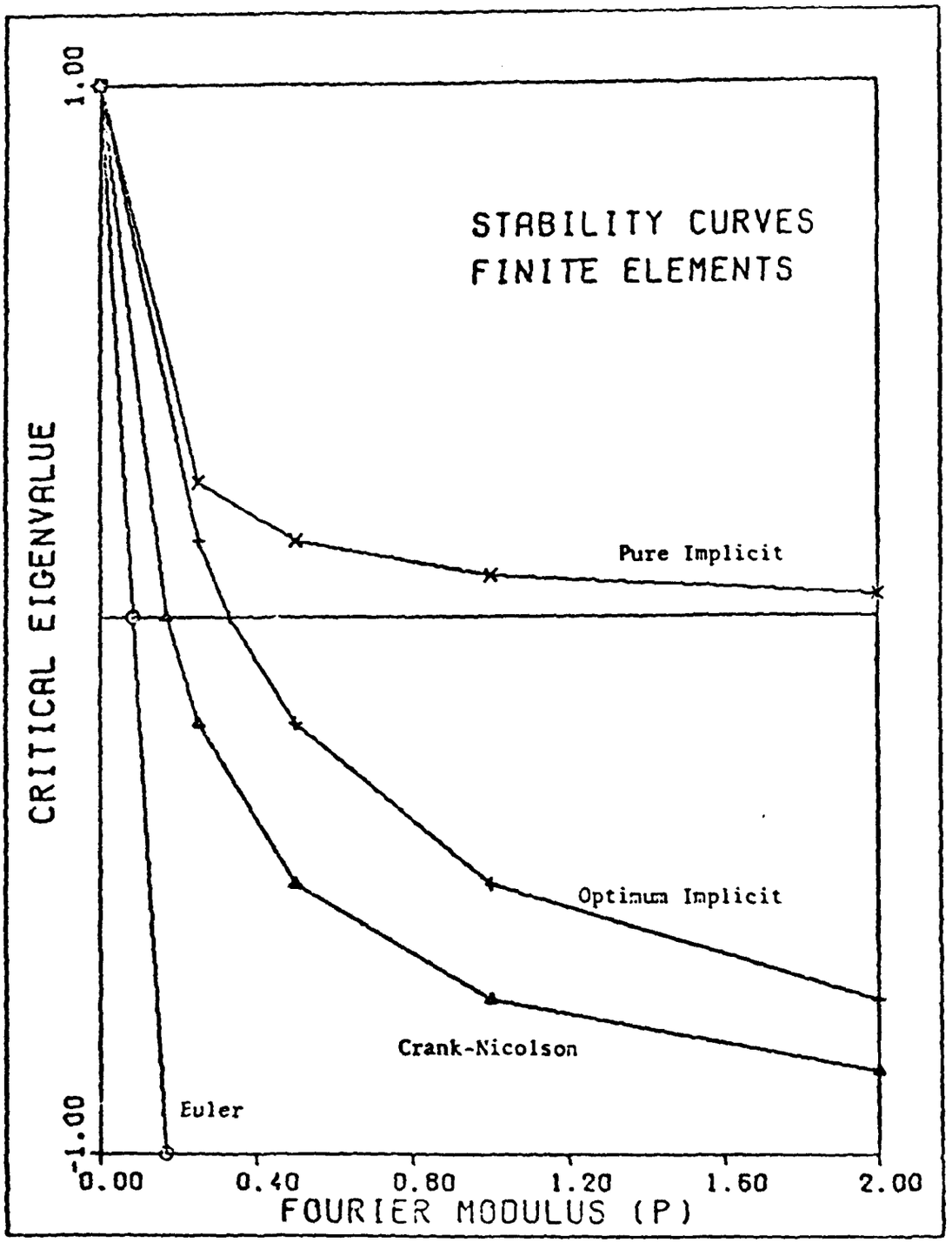
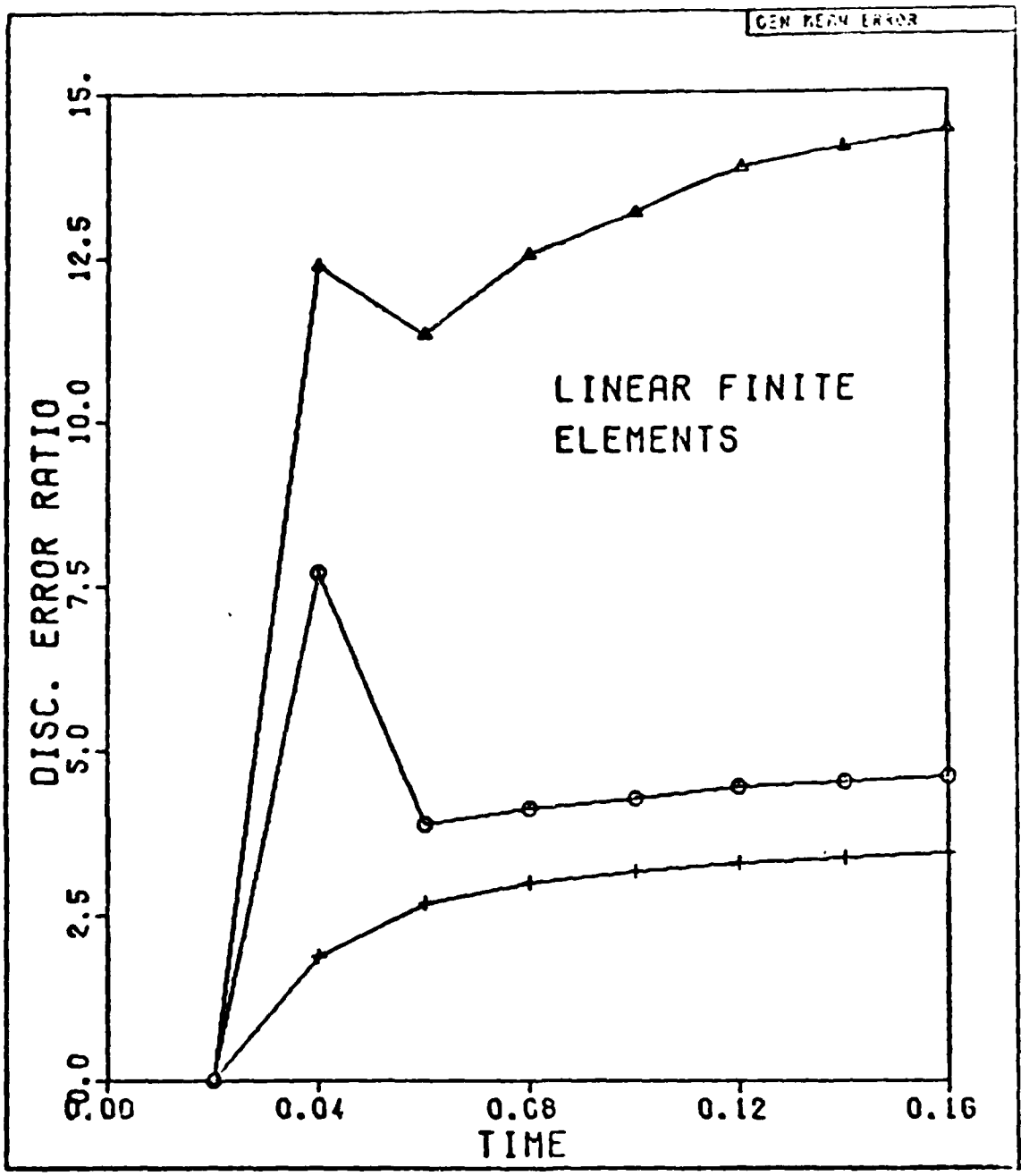


Figure 1. Stability Curves for Finite Elements.



⊙ Crank-Nicolson Method, $\alpha = 0.5$

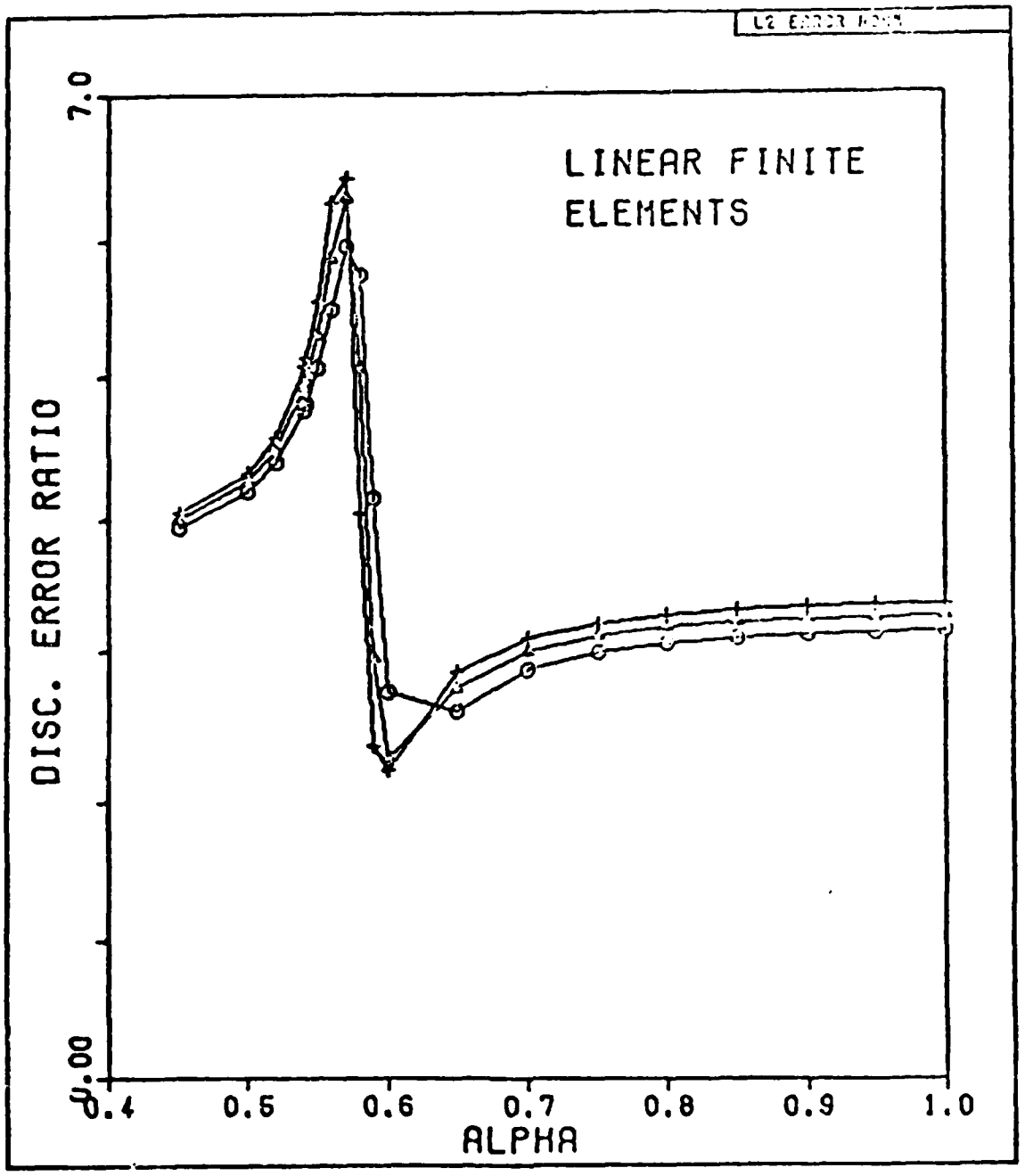
▲ Optimum Implicit Method, $\alpha = 0.5417$

\+ Pure Implicit Method, $\alpha = 1.0$

Fourier Modulus: $p = 2.0$

Discretization Change: $\Delta x = 0.1$ to $\Delta x = 0.05$

Figure 2. Convergence as a Function of Time for the truncation error.

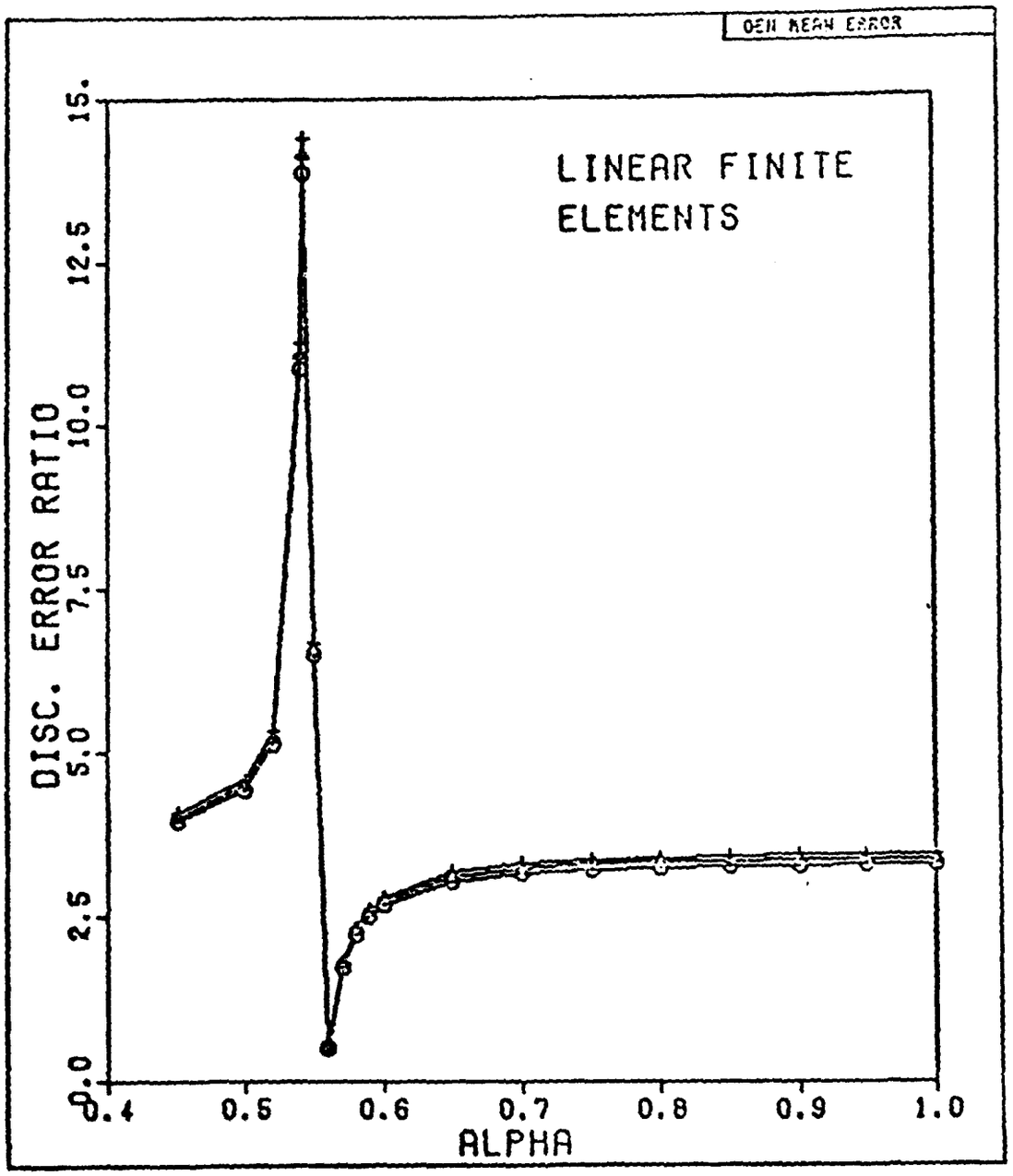


TIME ○ 0.12
△ 0.14
LEGEND: + 0.16

Fourier Modulus: p = 2.0

Discretization Change: $\Delta x = 0.1$ to $\Delta x = 0.05$

Figure 3. Convergence as a Function of α in the L_2 Norm.



TIME ○ 0.12

△ 0.14

LEGEND: + 0.16

Fourier Modulus: p = 2.0

Discretization Change: $\Delta x = 0.1$ to $\Delta x = 0.05$

Figure 4. Convergence as a function of α for the truncation error.

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